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Crossovers of the Density of States in Two-Direction Double-Barrier Resonant-Tunneling Structures

by

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Crossovers of the Density of States in Two-Direction Double-Barrier Resonant-Tunneling Structures

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Abstract

The density of states in delta-profiled 2D and 1D quantum systems is calculated. It is shown that there are smooth crossovers in the density of states from a 3D square-root behavior to a 2D steplike behavior, and from a 2D to a 1D sawtooth-like behavior, as the confinements increase.

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I. Introduction

Quantum-well structures are being extensively studied for applications in ultra-large-scale integrated circuits and high-speed optoelectronics. As for these systems, the lateral confinement of originally quasi-two-dimensional (Q2D) electron layers to submicron dimensions has made possible the realization of quasi-one-dimensional (Q1D) electron systems[1]. Among them, resonant-tunneling structures are of great interest not only because of their potential applications, but also for the underlying basic physics. A number of theoretical studies have been carried out recently[2-5]. For example, one of the authors has calculated the density of states and dwell times[3,4], and Bahder et al have calculated the local density of states for a simplified model with quite rigorous results[5].

Despite extensive investigations of quantum-well structures to date, we are not aware of any study of the cross sectional local density of states of a quantum-well wire structure. To solve this problem, we consider an artificial structure, the so-called two-direction double-barrier resonant-tunneling structure. In Section II we evaluate the eigenfunctions and eigenvalues from an effective-mass Schrödinger equation. For the delta-profiled potential model using these results in Section III, the local density of states has been determined. In Section IV, integrating over the well volume, we calculate the density of states in the well, where we show crossovers of the density of states from 3D to 1D via 2D.

II. Theoretical model

We consider a typical two-direction double-barrier resonant-tunneling structure (DBRTS) consisting of two thin (~ 50 Å) $Al_xGa_{1-x}As$ layers, separated by a thin GaAs layer in both directions. The potential is expressed by

$$V(y,x) = V_y(y) + V_z(z)$$
$$= V_1\{\delta(y+b) + \delta(y-b)\} + V_0\{\delta(z+a) + \delta(z-a)\} \quad . \qquad (1)$$

In this expression, the four $Al_xGa_{1-x}As$ potential barriers have been replaced by δ-functions with strengths V_1 and V_0 in the y- and z-direction, respectively. The parameter V_i (i = 0 or 1) is given by

$$V_i = d_i \Delta V_{ci} \quad , \qquad (2)$$

where d_i are the barrier widths and ΔV_{ci} are the conduction-band discontinuities. This additive potential form corresponds to a rectangular quantum wire with cross section a × b when V_1 and V_0 are very large and a and b are less than the deBroglie wavelength (λ_p) of the electron. The quantum wire with circular cross section also has a quasi-one-dimensional character, but the wavefunction in the confinement direction is the Bessel function.

We now solve the time-independend Schrödomger equation with the Hamiltonian

$$H = -\frac{\hbar^2}{2m_c}\nabla^2 + V(y,z) \quad , \qquad (3)$$

where m_c is the effective electron mass at the bottom of the GaAs conduction band. In order to deal with a finite density of states, we must take our structure within a large, impenetrable rigid box extended, say, from -L/2 to L/2. With these boundary conditions, the Schrödinger equation is separable with the additive potential form, and then we can write the wavefunction in the product form

$$\Psi(r) = L^{-1/2} \exp(ik_x x)\ \Psi(y)\Psi(z) \tag{4}$$

where $k_x = 2\pi n_x/L$ and n_x takes the integer values 0, 1, 2, ... The y- and z-parts of the wavefunction, $\Psi(y)$ and $\Psi(z)$, satisfy the reduced equations

$$\Psi''(y) + \frac{2m_c}{\hbar^2}\ [E_y - V(y)]\psi(z) = 0 \tag{5}$$

$$\Psi''(z) + \frac{2m_c}{\hbar^2}\ [E_z - V(z)]\psi(z) = 0 \quad , \tag{6}$$

where

$$E_y + E_z = E - \hbar^2 k_x^2/2m_c \quad . \tag{7}$$

Here, E is the total energy corresponding to the Hamiltonian H, and $E_y(E_z)$ is the energy eigenvalue of Eq. (5) ((6)). Because of the symmetry of our system, it is convenient to write the wavefunction in terms of even and odd functions as

$$\Psi_{ek_y}(y) = \begin{cases} A_1(k_y)\cos(k_y y) \quad , & 0 < y < b \\ \\ A_2(k_y)\cos(k_y y) + A_3(k_y)\sin(k_y y) \quad , & b < y < L/2 \end{cases} \tag{8}$$

and

$$\Psi_{ok_y}(y) = \begin{cases} B_1(k_y)\sin(k_y y) \quad , & 0 < y < b \\ B_2(k_y)\cos(k_y y) + B_3(k_y)\sin(k_y y) \quad , & b < y < L/2 \quad . \end{cases} \tag{9}$$

The z-components of the wavefunctions can be written in similar forms as

$$\Psi_{ek_z}(z) = \begin{cases} C_1(k_z)\cos(k_z z) \quad , & 0 < z < a \\ C_2(k_z)\cos(k_z z) + C_3(k_z)\sin(k_z z) \quad , & a < z < L/2 \end{cases} \tag{10}$$

and

$$\Psi_{ok_z}(z) = \begin{cases} D_1(k_z)\sin(k_z z) \quad , & 0 < z < a \\ D_2(k_z)\cos(k_z z) + D_3(k_z)\sin(k_z z) \quad , & a < z < L/2 \quad . \end{cases} \tag{11}$$

When we apply the boundary conditions to the y-components of the wavefunction, we get the equations for the bound states of even and odd parity, respectively, as

$$\frac{\gamma_1}{k_y}\cos(k_y b)\sin(k_y L/2 - k_y b) + \cos(k_y L/2) = 0 \tag{12}$$

and

$$\frac{\gamma_1}{k_y} \sin(k_y b)\sin(k_y L/2-k_y b) + \sin(k_y L/2) = 0 \quad , \tag{13}$$

where $\gamma_1 = 2m_c V_1/\hbar^2$. The coefficients A_i and B_i are

$$\frac{A_3}{A_1} = \frac{\gamma_1}{k_y} \cos^2(k_y b) \tag{14}$$

$$\frac{A_2}{A_1} = 1 - \frac{\gamma_1}{2k_y} \sin(2k_y b) \tag{15}$$

$$\frac{B_3}{B_1} = 1 + \frac{\gamma_1}{2k_y} \sin(2k_y b) \tag{16}$$

$$\frac{B_2}{B_1} = - \frac{\gamma_1}{k_y} \sin^2(k_y b) \quad . \tag{17}$$

With the same calculation for Eq. (6), we find similar results for the conditions of the bound states and coefficients C_i and D_i, by replacing b with a, k_y with k_z, and γ_1 with γ_0, which is $2m_c V_o/\hbar^2$. From the normalization conditions, A_1, B_1, C_1 and D_1 can be determined as shown for A_1 and B_1 in Ref. [5]. The energy eigenvalues corresponding to Eqs. (5) and (6) are given by

$$(E_{ky} + E_{kz})_\alpha = \frac{\hbar^2}{2m_c} (k_y^2 + k_z^2)_\alpha \quad , \tag{18}$$

where α (= e or o) labels the state's parity.

Taking γ_1 and γ_o both to be equal to zero, which is identical to the limit where the δ-functions are placed on the boundaries, that is, b = a = L/2, one recovers $A_3/A_1 = B_2/B_1 = C_3/C_1 = D_2/D_1 = 0$, $A_2/A_1 = B_3/B_1 = C_2/C_1 =$

$D_3/D_1 = 1$ and $A_1 = B_1 = C_1 = D_1 = (2/L)^{\frac{1}{2}}$, which is the result for the motion of a 3D particle in a rigid box.

III. Local density of states

The local density of states (DOS) in the DBRTS has been obtained in various cases [6]. It can be defined in the two-direction case as

$$N(y,z;E) = -\frac{2}{\pi} Im G(\vec{r},\vec{r};E)$$

$$= \frac{2}{L} \sum_{k_x} \sum_{\alpha\beta} \sum_{k_y k_z} |\Psi_{\beta k_y}(y)|^2 \, |\Psi_{\alpha k_z}(z)|^2 \, \delta(E-E_{\vec{k}}) \quad , \tag{19}$$

where the factor of 2 implies spin degeneracy, $G(\vec{r},\vec{r}';E)$ is the single-particle Green's function, and α and β (= e or o) label a state's partiy. When the system size goes to infinity, we can change the summation into the appropriate integration because the density of allowed wavevectors becomes $2\pi/L$:

$$N(y,z;E) = \frac{L^2}{2\pi^3} \int_0^\infty dk_x \delta(E-E_{\vec{k}}) \sum_\beta \int_0^\infty dk_y |\Psi_{\beta ky}(y)|^2 \sum_\alpha \int_0^\infty dk_z |\Psi_{\alpha kz}(z)|^2 \tag{20}$$

with

$$\sum_\beta |\Psi_{\beta ky}(y)|^2 = \frac{1}{2}[A_1^2 + B_1^2 + (A_1^2 - B_1^2)\cos(2k_y y)] \quad , \tag{21}$$

$$\sum_\alpha |\Psi_{\alpha kz}(z)|^2 = \frac{1}{2}[C_1^2 + D_1^2 + (C_1^2 - D_1^2)\cos(2k_z z) \quad . \tag{22}$$

Integrating Eq. (20) over k_x, we get

$$N(y,z;E) = \frac{L^2}{16\pi^3}\left(\frac{2m_c}{\hbar^2}\right)^{1/2}\int_0^\infty dk_y\ [A_1^2 + B_1^2 + (A_1^2 - B_1^2)\cos(2k_y y)]$$

$$\times \int_0^\infty dk_z\ \frac{[C_1^2 + D_1^2 + (C_1^2 - D_1^2)\cos(2k_z z)]}{[E - [\hbar^2/2m_c](k_y^2+k_z^2)]^{1/2}} \quad . \tag{23}$$

The wavefunction coefficients A_1, B_1, C_1 and D_1 are given by

$$\lim_{2b/L\to 0} (L/2)A_1^2[p/b] = \frac{p^2}{p^2 + U_1^2\cos^2(p) - U_1\ p\ \sin(2p)} = F_e(p) \tag{24a}$$

$$\lim_{2b/L\to 0} (L/2)B_1^2(p/b) = \frac{p^2}{p^2 + U_1^2\sin^2(p) + U_1\ p\ \sin(2p)} = F_o(p) \tag{24b}$$

$$\lim_{2b/L\to 0} (L/2)C_1^2(q/a) = \frac{q^2}{q^2 + U_o^2\cos^2(q) - U_o\ q\ \sin(2q)} = G_e(q) \tag{24c}$$

$$\lim_{2a/L\to 0} (L/2)D_1^2(q/a) = \frac{q^2}{q^2 + U_o^2\sin^2(q) - U_o\ q\ \sin(2q)} = G_o(q) \tag{24d}$$

where $p = k_y b$, $q = k_z a$, $U_1 = \gamma_1 b$ and $U_o = \gamma_o a$. Furthermore, when we allow V_1 or V_0 to go to zero, $N(y,z';E)$ becomes $N(z;E)$ or $N(y;E)$, which is that of the one-direction DBRTS.

Equation (23) shows the cross-sectional local DOS of the quantum-well wire, the so-called two-direction DBRTS, which consists of two parts, each

coming from even and odd parity, respectively. In both the y- and z-directions, it shows sinusoidal behavior. In the limit of $V_1 \to 0$ and $V_0 \to 0$, the functions F(p) and G(q) are unity and N(y,z;E) becomes the DOS of a free electron in a box of volume 4abL.

IV. Crossovers of the density of states

We now consider the DOS in the well, N(E), which can be calculated by taking the integral over the well volume.

$$N(E) = 8 \int_0^{L/2} \int_0^b \int_0^a dx\, dy\, dz\, N(y,z;E) \quad . \tag{25}$$

The result is

$$N(E) = \frac{L2m_c}{\pi^3\hbar^2} \int_0^{b\eta} dp\ [F_e(p) + F_o(p) + (F_e(p)-F_o(p))\sin(2p)/2p]$$

$$\times \int_0^{a(\eta^2-(p/b)^2)^{1/2}} dq\ [\frac{G_e(q) + G_o(q) + (G_e(q)-G_o(q))\sin(2q)/2q}{(\eta^2 - (q/a)^2 - (p/b)^2)^{1/2}}] \quad , \tag{26}$$

where $\eta^2 = 2m_c E/\hbar^2$.

Let us evaluate the DOS for a few extreme cases.

(i) 3D case

This corresponds to the limits $U_1 \ll 1$ and $U_o \ll 1$, i.e., $F_e(p) = F_o(p) = G_e(q) = G_o(q) = 1$. Then we arrive at

$$N(E) = \frac{8m_c L}{\pi^3\hbar^2} \int_0^{b\eta} dp \int_0^{a(\eta^2-(p/b)^2)^{1/2}} dq\ 1/(\eta^2-(q/a)^2-(p/b)^2)^{1/2}$$

$$= \frac{1}{2\pi^2}\, 4abL\, \frac{2m_c}{\hbar^2}\, E^{1/2} \quad . \tag{27}$$

which is the well-known DOS of a 3D free-electron gas with volume 4abL.

(ii) 2D case

In this case, either U_1 or U_0 goes to zero while the other goes to infinity, i.e., $U_o \to \infty$ and $U_1 \to 0$ or vice versa, such that Eq. (26) becomes

$$N(E) = \frac{4Lm_c}{\pi^3\hbar^2} \int_0^{b(\eta^2-(q/a)^2)^{1/2}} dp\ 1/(n^2-(p/b)^2-(q/a)^2)^{1/2}$$

$$\times \int_0^{a\eta} dq\ [G_e(q) + G_o(q) + (G_e(q) - G_o(q))\sin(2q)/2q] \quad . \tag{28}$$

For $U_o \to \infty$, the DOS becomes

$$N(E) = \frac{4Lm_c b}{2\pi\hbar^2} \sum_{n=0}^{\infty} \int_0^{a\eta} dq\Big[\delta(q-(n+1/2)\pi + \delta(q-(n+1)\pi) + [\delta(q-(n+1/2)\pi)$$

$$- \delta(q-(n+1)\pi)]\ [\sin(2q)/2q]\Big]$$

$$= \frac{m_c 2bL}{\hbar^2\pi} \sum_{n=0}^{\infty} \int_0^{a\eta} dq[\delta(q-(n+1/2)\pi) + \delta(q-(n+1)\pi)]$$

$$= \frac{m_c 2bL}{\hbar^2\pi} \sum_{n=1}^{\infty} \Theta(E-n^2E_o) \quad , \tag{29}$$

where Θ is the unit step function and $E_o = \pi^2\hbar^2/(8m_c a^2)$. Here, we have used the fact that $G_\alpha(q)$ can be represented in terms of δ-functions when U_0 goes to infinity (see Fig. 1).

(iii) 1D case

This corresponds to U_0 and U_1 both going to infinity so as to confine the motion of the electrons to just one direction:

$$N(E) = \frac{L2m_c}{\pi^3\hbar^2}\int_0^{b\eta} dp\ \pi \sum_{m=0}^{\infty} [\delta(p-(m+1/2)\pi) + \delta(p-(m+1)\pi)]$$

$$\times \sum_{n=0}^{\infty} \int_0^{a(\eta^2-(p/b)^2)1/2} dq\ \frac{\pi[\delta(q-(n+1/2)\pi) + \delta(q-(n+1)\pi)]}{[\eta^2 - (q/a)^2 - (p/b)^2]^{1/2}}$$

$$= \frac{L}{\pi}\left(\frac{2m_c}{\hbar^2}\right)^{1/2} \sum_{m,n}^{\infty} \Big[1/[E-(\hbar^2\pi^2 2m_c)(((m+1/2)/b)^2 + ((n+1/2)/a)^2)]^{1/2}$$

$$+ 1/[E-(\hbar^2\pi^2/2m_c)(((m+1/2)/b)^2 + ((n+1)/a^2)]^{1/2}$$

$$+ 1/[E-(\hbar^2\pi^2/2m_c)(((m+1)/b)^2 + ((n+1/2)/a)^2)]^{1/2}$$

$$+ 1/[E-(\hbar^2\pi^2/2m_c)(((m+1)/b)^2 + ((n+1)/a))]^2)]^{1/2}\Big] \qquad (30)$$

We have again used the fact that $F_\alpha(p)$ behaves as δ-function when U_1 goes to ∞.

In order to find the crossovers of the DOS in the well from 3D to 2D graphically, we modify Eq. (26) as

$$\frac{\pi^2\hbar^2}{2bLm_c} N(E) = \int_0^{\pi/2(E/E_o)^{1/2}} dq\ [G_e(q) + G_o(q) + \{G_e(q)-G_o(q)\}\sin(2q)/2q] \quad , \tag{31}$$

where $\pi/2(E/E_o)^{1/2} = a\eta$ and $G_\alpha(q)$ is given by Eqs. (24c) and (24d). Similarly, the equation which shows that the crossovers of the DOS in the well from 2D to 1D is expressed as

$$\frac{\pi^2\hbar^2}{2Lm_c} N(E) = \sum_{m=0}^{\infty} \int^{\pi/2(E/E_o)^{1/2}} dq[G_e(q) + G_o(q) + \{G_e(q)-G_o(q)\}\sin(2q)/2q]$$

$$\times \frac{1}{[(\pi/2a)^2 E/E_o - \{(m+1/2)\pi/b\}^2 - (q/a)^2]^{1/2}}$$

$$\left. + \frac{1}{[(\pi/2a)^2 (E/E_o) - \{(m+1)\pi/b\}^2 - (q/a)^2]^{1/2}} \right] \quad . \tag{32}$$

Figure 2 shows the graphical result of Eq. (31), namely, the crossovers of the DOS in the well from 3D to 2D. In this case we take $U_1 = 0$, U_o changes from 0 to 20, and E/E_o varies from 0 to 8. On the other hand, Fig. 3 shows the transition of the DOS in the well from 2D to 1D. For the sake of convenience, we take $a = b$, U_1 to go to infinity, and U_o to vary from 0 to 20. Higher values of U_o correspond to increased sharp peaks of the DOS of the 1D, quantum-wire case. In this case, our result recovers the well-known sawtooth type DOS diverging at values of $E/E_o = 2, 5, 8, 10, \ldots$, which is in good agreement with Arakawa and Sakaki[7]. The values at 5 and 10 are roughly

twice those at 2 and 8, respectively, which comes from the double degeneracy of the eigenstates.

V. Concluding remarks

Considering a quantum wire with a rectangular cross-section of $a \times b$ and very long length L, which may be called a two-direction DBRTS when the confining potential is not very high, within a very large box of volume L^3, we have calculated the local DOS and DOS in the well. The latter shows crossovers from a 3D square-root behavior to a 1D sawtooth-type behavior, via a 2D staircase-like behavior, when the confining potential is very high ($U_i \gg 1$). The higher values of U_1 in the case of the transition from 2D to 1D correspond to increased sharp peaks and finally reach the ideal sawtooth-type behavior with singularities at the values of $E/E_o = 2, 5, 8, 10, \ldots$ If we consider a small quantum box of volume $a \times b \times c$ in a large box of volume L^3, we see a transition of a finite DOS from 1D to 0D which is expressed as a sum of delta functions [7].

Although our calculations have been performed so far for rather artificial delta-profiled systems only, we are quite positive that this kind of DOS transition will also occur in real systems where, for example, the barriers have finite widths. For barriers with finite thickness, the effective mass of the electron changes in passing from the quantum well region (GaAs) to the barrier regions (AlGaAs) of the structure. For this, BenDaniel and Duke [8] suggest that current conservation is guaranteed on both sides by use of the boundary condition

$$\frac{1}{m_1}\frac{\partial \Psi}{\partial z} = \frac{1}{m_2}\frac{\partial \Psi}{\partial z} , \qquad (33)$$

where m_1 and m_2 are the effective masses of GaAs and AlGaAs, respectively. Also, Bruno and Bahder [6] have considered this for the one-direction DBRTS case and showed that the DOS at the low-energy subband edges is higher than the DOS would be at the same energies in the absence of barriers (for delta-profiled barriers). So for our two-direction DBRTS case, we can estimate that our result for the DOS will also be increased a bit upward at the same energies because of the additive form of the potential which we have taken. Additive forms of potentials are used to describe the motion of an electron in parabolic quantum wires [9] or quantum boxes [10]. Even if we take a quantum wire with circular cross section, the wavefunctions are expressed in a different way with Bessel functions, but the main feature of our calculation will not change much.

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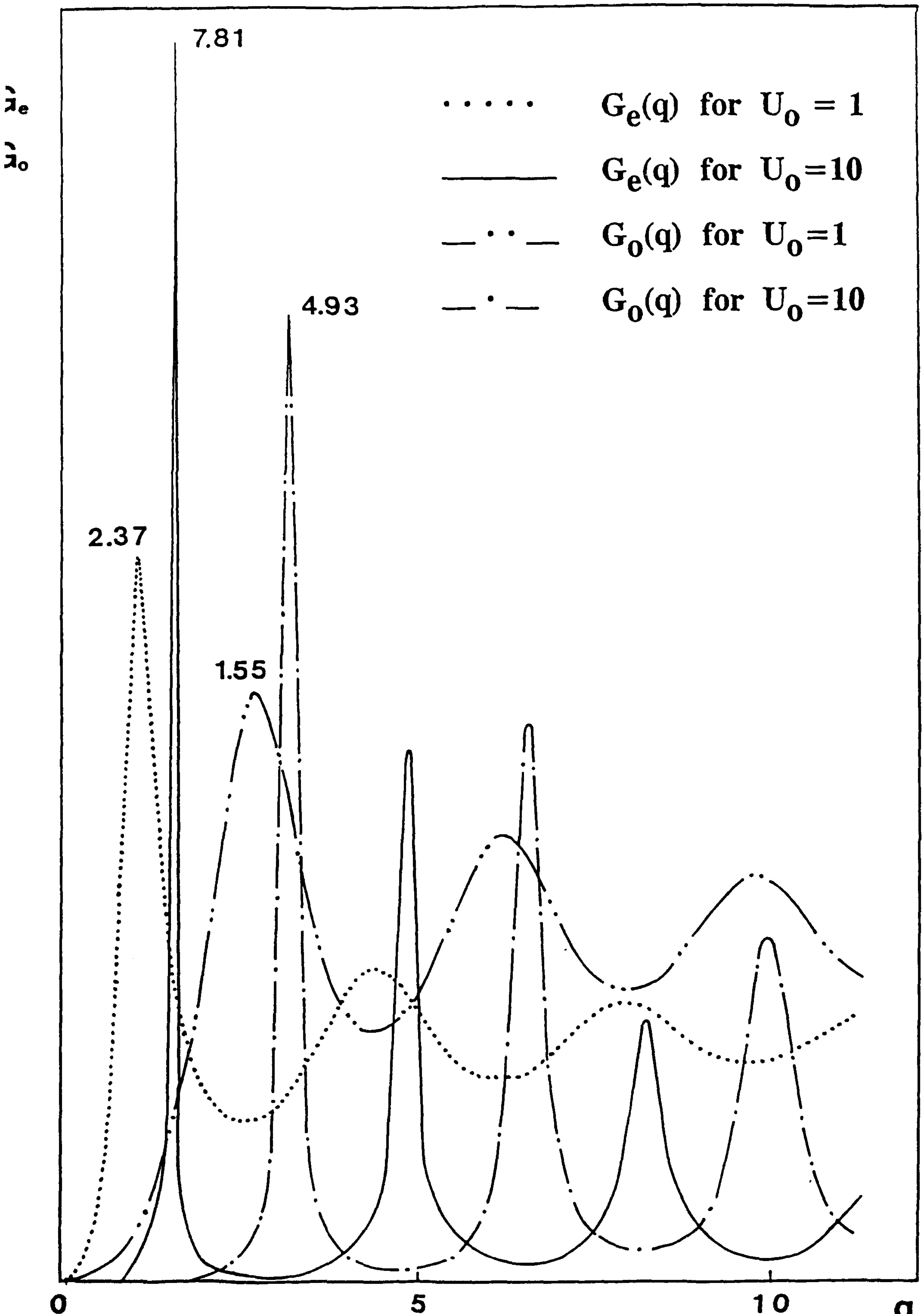
Figure Captions

1. Behaviors of $G_e(q)$ and $G_o(q)$ for $U_o = 1$ and $U_o = 10$.

2. Crossover of the ~~global~~ DOS in the well from 3D to 2D in the range from $U_o = 0$ to $U_o = 20$, i.e., $\frac{\pi^2\hbar^2}{2bLm_c}N(E)$ as a function of $\frac{E}{E_o}$. Here U_o takes the values 0, 2, 12, 16, 20.

3. Crossover of the ~~global~~ DOS in the well from 2D to 1D. Here we take $U_1 = \infty$ and $U_o = 0, 2, 8, 16, 20$. Higher values of U_0 correspond to a sawtooth-like 1D behavior.



Ge
Go
7.81
4.93
2.37
1.55
· · · · · $G_e(q)$ for $U_0 = 1$
$G_e(q)$ for $U_0=10$
$G_0(q)$ for $U_0=1$
$G_0(q)$ for $U_0=10$
0
5
10
q

Fig. 1

Fig. 2

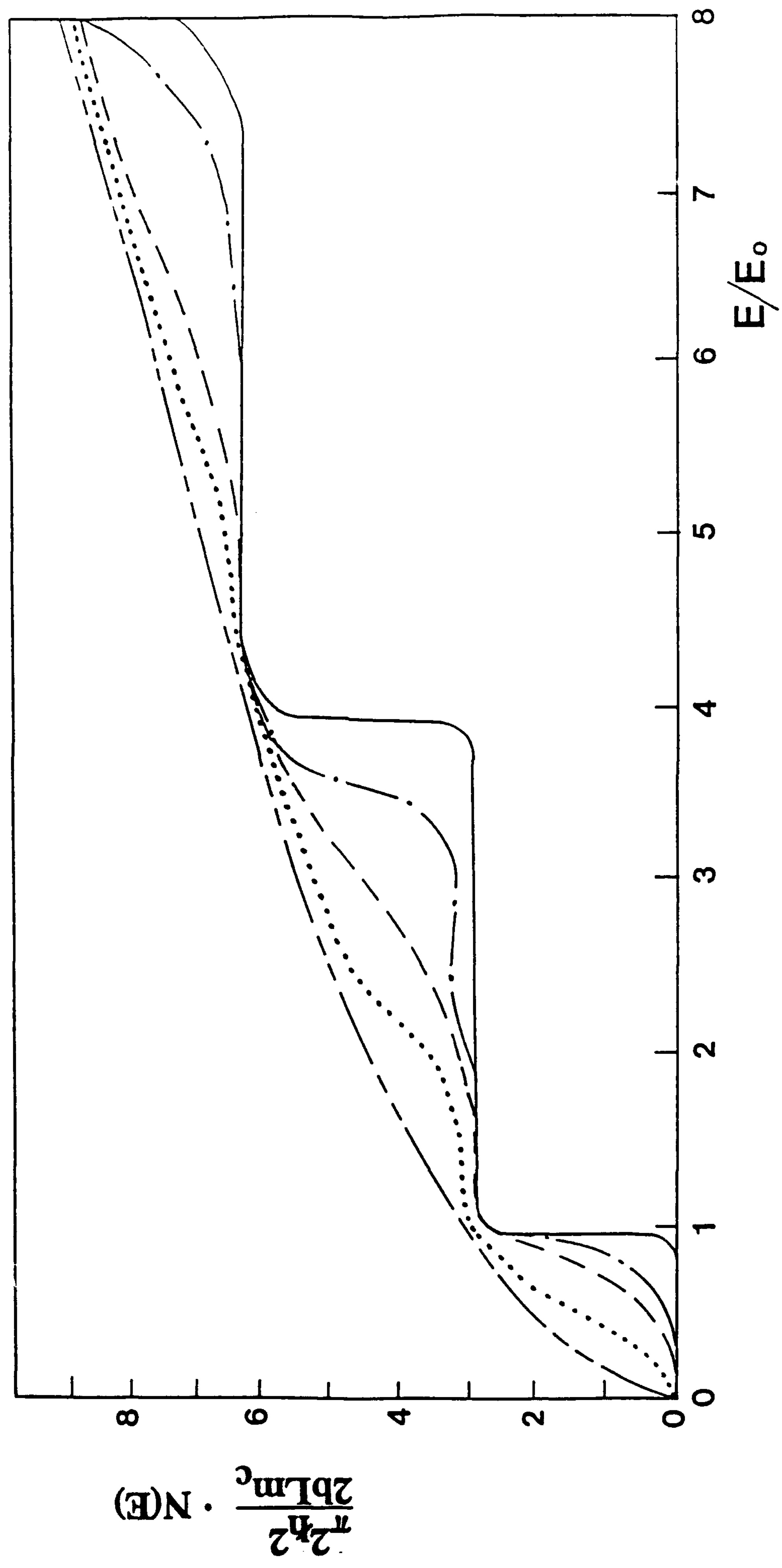


Fig. 3